MACROSCOPIC-MICROSCOPIC MASS MODELS

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Abstract: We discuss recent developments in macroscopic-microscopic mass models, including the 1992 finite-range droplet model, the 1992 extended-Thomas-Fermi Strutinsky-integral model, and the 1994 Thomas-Fermi model, with particular emphasis on how well they extrapolate to new regions of nuclei. We also address what recent developments in macroscopic-microscopic mass models are teaching us about such physically relevant issues as the nuclear curvature energy, a new congruence energy arising from a greater-than-average overlap of neutron and proton wave functions, the nuclear incompressibility coefficient, and the Coulomb redistribution energy arising from a central density depression. We conclude with a brief discussion of the recently discovered rock of metastable superheavy nuclei near $^{272}110$ that had been correctly predicted by macroscopic-microscopic models, along with a possible new tack for reaching an island near $^{290}110$ beyond our present horizon.

1. Introduction

The accurate calculation of the ground-state mass and deformation of a nucleus, specified by its proton number Z and neutron number N, remains a fundamental challenge of nuclear theory. Approaches developed over the years to achieve this difficult yet all-important goal span a broad spectrum: (1) fully selfconsistent microscopic theories starting with an underlying nucleon-nucleon interaction, (2) macroscopic-microscopic models utilizing calculated shell and pairing corrections, (3) mass formulas with empirical shell terms whose parameters are extracted from adjustments to experimental masses, (4) algebraic expressions based on the nuclear shell model, and (5) neural networks.

At the most fundamental of the above levels, microscopic theories have seen progress in both the nonrelativistic Hartree-Fock approximation[1)] and more recently the relativistic mean-field approximation.[2–6)] Important steps have also been taken to construct an effective Lagrangian

Figure 1: Comparison of experimental and calculated microscopic corrections for the original 1654 nuclei included in the 1992 adjustment of the finite-range droplet model.[10,11] The difference between these two quantities shown in the bottom part of the figure is equivalent to the difference between experimental and calculated masses.

for use in such theories based on the chiral symmetry of quantum chromodynamics.[7–9] Microscopic theories offer great promise for the future, but so far have been applied only to limited regions of mainly spherical nuclei, with accuracies that are typically a few MeV. For example, the average absolute deviation between the calculated and experimental masses of 32 spherical nuclei that were considered in one relativistic treatment[4] is 2.783 MeV.

At the second level of fundamentality, the macroscopic-microscopic method—where the smooth trends are obtained from a macroscopic model and the local fluctuations from a microscopic model—has been used in several recent global calculations. We will concentrate here on three such calculations,[10–15] with particular emphasis on how well they extrapolate to new regions of nuclei, but will also include an example of each of the remaining approaches.[16–18] We will then discuss some new physical insight provided by macroscopic-microscopic mass models, and conclude with their prediction of the recently discovered rock of metastable superheavy nuclei near $^{272}110$ and of an island near $^{290}110$ beyond our present horizon.

2. Finite-Range Droplet Model

In the finite-range droplet model, which takes its name from the macroscopic model that is used, the microscopic shell and pairing corrections are calculated from a realistic, diffuse-surface, folded-Yukawa single-particle potential by use of Strutinsky's method.[19] In 1992 we made a new adjustment of the constants of an improved version of this model[10,11] to 28 fission-barrier heights and to 1654 nuclei with $N, Z \geq 8$ ranging from ^{16}O to $^{263}106$ whose masses were known experimentally in 1989.[20] The resulting microscopic corrections are shown in Fig. 1.

Figure 2: Theoretical error as a function of mass number for the original 1654 nuclei included in the 1992 adjustment of the finite-range droplet model.[10,11] The dashed line shows the constant value 0.669 MeV appropriate to the entire region of nuclei considered.

The improvements include minimization of the nuclear potential energy of deformation with respect to ϵ_3 and ϵ_6 shape degrees of freedom in addition to the usual ϵ_2 and ϵ_4 deformations, use of the Lipkin-Nogami extension of the BCS method for calculating the pairing correction, use of a new functional form and optimized constant for the effective-interaction pairing gap, use of ground-state single-particle levels calculated for each nucleus individually, use of an eighth-order Strutinsky shell correction with basis functions containing 12 oscillator shells, and inclusion of a zero-point energy in the quadrupole degree of freedom only. This model has been used to calculate the ground-state masses, deformations, odd-particle spins, pairing gaps, separation energies, and other properties for 8979 nuclei with $N, Z \geq 8$ ranging from ^{16}O to ^{339}136 and extending from the proton drip line to the neutron drip line.[10,11]

For the original 1654 nuclei included in the adjustment, the theoretical error, determined by use of the maximum-likelihood method with no contributions from experimental errors,[10,11] is 0.669 MeV. As can be seen in the bottom part of Fig. 1, some large systematic errors are still present for light nuclei but decrease significantly for heavier nuclei. The decrease in theoretical error with increasing mass number is presented quantitatively in Fig. 2. Each solid circle gives the theoretical error for a region extending 24 mass units below it and 25 mass units above it. These points are well represented by the function 8.62 MeV$/A^{0.57}$ shown by the solid line.

3. Extrapolateability to New Regions of Nuclei

Between 1989 and 1993, the masses of 217 additional nuclei heavier than ^{16}O have been measured,[21] which provides an ideal opportunity to test the ability of mass models to extrapolate to new regions of nuclei whose masses were not included in the original adjustment.

Figure 3: Deviations between experimental and calculated masses for 217 new nuclei whose masses were not included in the 1992 adjustment of the finite-range droplet model.[10,11]

Figure 3 shows as a function of the number of neutrons from β-stability the individual deviations between these newly measured masses and those predicted by the 1992 finite-range droplet model. The theoretical error for these 217 newly measured masses is 0.642 MeV, corresponding to a *decrease* of 4%. This model can therefore be extrapolated to new regions of nuclei with considerable confidence.

Analogous deviations are shown in Fig. 4 for the 1992 Thomas-Fermi Strutinsky-integral model (version 1) of Aboussir, Pearson, Dutta, and Tondeur.[12] In this model, the macroscopic energy is calculated for a Skyrme-like nucleon-nucleon interaction by use of an extended Thomas-Fermi approximation. The shell correction is calculated from single-particle levels corresponding to this same interaction by use of a Strutinsky-integral method, and the pairing correction is calculated for a δ-function pairing interaction by use of the conventional BCS approximation. The constants of the model were determined by adjustments to the ground-state masses of 1492 nuclei with mass number $A \geq 36$, which excludes the troublesome region from ^{16}O to mass number $A = 35$. The theoretical error corresponding to 1538 nuclei whose masses were known experimentally[20] at the time of the original adjustment is 0.726 MeV. The theoretical error for 210 newly measured masses[21] for nuclei with $A \geq 36$ is 0.810 MeV, corresponding to an increase of 12%. Some caution should therefore be exercised when extrapolating this model to new regions of nuclei.

Similar results are shown in Fig. 5 for the 1994 Thomas-Fermi model of Myers and Swiatecki. In this model,[13–15] the macroscopic energy is calculated for a generalized Seyler-Blanchard nucleon-nucleon interaction by use of the original Thomas-Fermi approximation. For $N, Z \geq 30$ the shell and pairing corrections were taken from the 1992 finite-range droplet model, and for $N, Z \leq 29$ a semi-empirical expression was used. The constants of the model were determined

Figure 4: Deviations between experimental and calculated masses for 210 new nuclei whose masses were not included in the 1992 adjustment of the extended-Thomas-Fermi Strutinsky-integral model.[12)]

Figure 5: Deviations between experimental and calculated masses for 217 new nuclei whose masses were not included in the 1994 adjustment of the Thomas-Fermi model.[13–15)]

Table 1: Extrapolateability to New Regions of Nuclei.

Model	Original nuclei $N_{\rm nuc}$	Original nuclei Error (MeV)	New nuclei $N_{\rm nuc}$	New nuclei Error (MeV)	Error ratio
FRDM (1992)	1654	0.669	217	0.642	0.96
ETFSI-1 (1992)	1538	0.726	210	0.810	1.12
TF (1994)	1654	0.640	217	0.737	1.15
v. Groote (1976)	1323	0.629	217	1.284	2.04

by adjustments to the ground-state masses of the same 1654 nuclei with $N, Z \geq 8$ ranging from ^{16}O to ^{263}106 whose masses were known experimentally in 1989 that were used in the 1992 finite-range droplet model. The theoretical error corresponding to these 1654 nuclei is 0.640 MeV. The reduced theoretical error relative to that in the 1992 finite-range droplet model arises primarily from the use of semi-empirical microscopic corrections in the extended troublesome region $N, Z \leq 29$ rather than microscopic corrections calculated more fundamentally. The theoretical error for 217 newly measured masses[21)] is 0.737 MeV, corresponding to an increase of 15%. Some caution should again be exercised when extrapolating this model to new regions of nuclei.

These theoretical errors are summarized in Table 1, where we also include—because of its frequent use in astrophysical calculations—the 1976 mass formula of von Groote, Hilf, and Takahashi.[16)] For this mass formula with empirical shell terms whose parameters are extracted from adjustments to experimental masses, the theoretical error for 217 newly measured masses[21)] increases by 104% relative to the theoretical error for 1323 nuclei whose masses were known experimentally in 1977. This formula extrapolates to new regions of nuclei very poorly and is therefore inappropriate for use in modern-day astrophysical calculations.

For the recent mass formula of Duflo and Zuker,[17)] which is an example of an algebraic expression based on the nuclear shell model, the increase in root-mean-square error for newly measured masses relative to that for masses included in the original adjustment is 32%. Finally, for one particular neural network of Gernoth, Clark, Prater, and Bohr that had not been pruned for improved extrapolateability,[18)] the increase in root-mean-square error for newly measured masses relative to that for masses included in the original training is 772%. These last two examples are not included in Table 1 because the regions of newly measured masses are different from those in the table and because we have available only the root-mean-square errors, which are contaminated by contributions from experimental errors.

4. New Physical Insight

Recent developments in macroscopic-microscopic mass models are also providing new insight in several areas, including the nuclear curvature energy, a new congruence energy, the nuclear

incompressibility coefficient, and the Coulomb redistribution energy. Myers and Swiatecki offer a simple resolution of the long-standing nuclear-curvature-energy anomaly[22] in terms of their 1994 Thomas-Fermi model.[13–15] This model is characterized by a curvature-energy constant $a_3 = 12.1$ MeV but nevertheless adequately reproduces nuclear ground-state masses through the counteraction of terms that are of still higher order in $A^{-1/3}$. The fission barriers of medium-mass nuclei calculated with such a large curvature-energy constant have in the past been significantly higher than experimental values, but in their view the shape dependence of a new congruence energy arising from a greater-than-average overlap of neutron and proton wave functions[23] resolves this difficulty.

The value of the incompressibility coefficient K adopted in the 1992 finite-range droplet model[10,11] from a variety of considerations is 240 MeV. An adjustment of K in this model to optimally reproduce both ground-state masses and fission-barrier heights gives 243 MeV, although this adjustment is not able to rule out values of K in the range from somewhat below 200 MeV to about 500 MeV. The value of K determined in the 1992 extended-Thomas-Fermi Strutinsky-integral model[12] is 234.7 MeV and that determined in the 1994 Thomas-Fermi model[13–15] is 234 MeV. However, these values are also subject to large uncertainties.

The inclusion of ϵ_3 and ϵ_6 shape degrees of freedom in the finite-range droplet model permitted the isolation of the Coulomb redistribution energy, in which the nuclear ground-state mass is lowered through the development of a central depression in the nuclear charge density.[24] This effect also appears naturally in other macroscopic models such as the 1992 extended-Thomas-Fermi model[12] and the 1994 Thomas-Fermi model[13–15]. The magnitude of this energy, which is several MeV for a heavy nucleus, increases strongly with increasing proton number. Consequently, models that do not take it into account are likely to be seriously in error when making predictions for superheavy nuclei.

5. Rock of Metastable Superheavy Nuclei

Several macroscopic-microscopic mass models[25–30] predict a rock of deformed metastable superheavy nuclei near $^{272}110$, in addition to an island of superheavy nuclei associated with the more familiar spherical magic proton number $Z = 114$ and neutron number $N = 184$. As illustrated in Fig. 6, the underlying physical origin of this rock of deformed superheavy nuclei is the development of large gaps in the single-particle energies at proton number $Z = 104$, 106, 108, and 110 and at neutron number $N = 162$ and 164 for prolate deformations in the vicinity of $\epsilon_2 = 0.2$.

Because superheavy nuclei can decay by either spontaneous fission, alpha decay, or beta decay (including electron capture), all of these decay modes must be considered when calculating their half-lives. The spontaneous-fission half-life depends upon both the fission barrier and the inertia for motion in the fission direction. This inertia can be calculated by use of either a microscopic cranking model or a semi-empirical relationship involving the irrotational inertia. The half-lives for alpha decay and beta decay depend primarily upon the corresponding energy

Figure 6: Dependence of single-proton and single-neutron energies upon deformation[10,11] for the metastable superheavy nucleus $^{272}110$.

releases Q_α and Q_β, which are given by appropriate differences of ground-state masses. When all decay modes are considered, the longest-lived spherical superheavy nuclei are those near $^{290}110$, with predicted half-lives of the order of years. The deformed superheavy nuclei near $^{272}110$ are predicted to have shorter half-lives of the order of milliseconds.[25–30]

Deformed metastable superheavy nuclei near $^{272}110$ have recently been discovered[31–36] through reactions of the type illustrated in Fig. 7. In the cold-fusion reactions involving nearly magic spherical targets utilized at the Gesellschaft für Schwerionenforschung in Darmstadt, Germany, the excitation energy is sufficiently low that the compound nuclei produced can de-excite to their ground states by the emission of a single neutron.[31–33] In contrast, in the hot-fusion reactions involving deformed targets utilized at the Joint Institute for Nuclear Research in Dubna, Russia by a Dubna-Livermore team, the excitation energy is sufficiently high that the compound nuclei produced must de-excite to their ground states by the emission of some five neutrons.[34–36]

Ingenius new tacks will be required to reach the island of spherical superheavy nuclei near $^{290}110$ that is predicted to lie beyond our present horizon. One possibility involves the use of prolately deformed targets and projectiles that also possess large negative hexadecapole moments, which leads to large waistline indentations.[37] When such nuclei collide with their symmetry axes perpendicular to each other, the resulting configurations are very compact, and little additional energy should be required to drive the system inside its fission saddle point.

Reactions between such nuclei might provide a path to the far side of the superheavy island.

6. Conclusion

Three macroscopic-microscopic models have been used recently to calculate the ground-state masses and deformations of nuclei throughout our known chart and beyond. One of these models can be extrapolated to new regions of nuclei whose masses were not included in the original adjustment with considerable confidence, and the other two can be extrapolated to new regions when some caution is exercised. Recent developments in these models are providing new physical insight in several areas. Macroscopic-microscopic models have also correctly predicted the existence and location of a rock of deformed metastable superheavy nuclei near $^{272}110$ that has recently been discovered. Nuclear ground-state masses and deformations will continue to provide an invaluable testing ground for nuclear many-body theories. The future challenge is for the fully microscopic theories to predict these quantities with comparable or greater accuracy.

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Figure 7: Calculated microscopic correction[10,11] in the vicinity of the recently discovered rock of metastable superheavy nuclei near $^{272}110$. An island near $^{290}110$ beyond our present horizon is also predicted by these calculations.

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